

4-(Chloromethyl)-2-ethoxy-1,3,2lambda⁵-dioxaphospholan-2-one

67554-11-4 | DTXSID50791173

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.14 days

Global applicability domain: Outside

Local applicability domain index: 8.08e-02

Confidence level: 8.16e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Methylhexane</div> <div>Measured: 3.00</div> <div>Predicted: 5.54</div>	<div>Image not found</div> <div>2-Methylheptane</div> <div>Measured: 3.00</div> <div>Predicted: 3.99</div>	<div>Image not found</div> <div>3-Methylhexane</div> <div>Measured: 9.00</div> <div>Predicted: 6.83</div>
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